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DOI: <https://doi.org/10.1007/s00791-004-0146-z>

Posted at the Zurich Open Repository and Archive, University of Zurich

ZORA URL: <https://doi.org/10.5167/uzh-21766>

Journal Article

Originally published at:

Babuska, I; Sauter, Stefan A (2004). Efficient solution of lattice equations by the recovery method. I. Scalar elliptic problems. *Computing and Visualization in Science*, 7(3-4):113-119.

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Efficient Solution of Lattice Equations by the Recovery Method.

Part I: Scalar Elliptic Problems

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November 8, 2002

Abstract

In this paper, an efficient solver for high-dimensional lattice equations will be introduced. We will present a new concept, the *recovery method*, to define a bilinear form on the continuous level which has equivalent energy as the original lattice equation. The finite element discretisation of the continuous bilinear form will lead to a stiffness matrix which serves as an quasi-optimal preconditioner for the lattice equations. Since a large variety of efficient solvers are available for linear finite element problems the new recovery method allows to apply these solvers for unstructured lattice problems.

1 Introduction

Lattice models are used in many applications such as models of heterogeneous materials ([22], [10]), fracture models ([23]), porous media ([7], [6]), biophysics ([17]). For a survey of some applications, we refer to [22] and [24]. Lattices are becoming more and more interesting for industrial production because these materials are light, cheap, and can be designed to prescribed stiffness requirements.

Periodic lattices in \mathbb{R}^n have been analysed in various papers by the Fourier transform and by Green's function (see, e.g., [11], [18], [21], [2]). This approach allows to analyse theoretical questions as the existence and uniqueness and also it was the basis for numerical treatments. Theoretical problems as the existence and uniqueness of the solution of general unbounded unstructured lattice equations have been analysed in [1] by using the ideas and results in the theory of partial differential equations of elliptic type.

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In this paper, we will develop a novel concept for the efficient solution of (finite) lattice equations. The efficient solution of unstructured lattice equations is not far developed in the literature yet. In contrast, the literature on solvers for finite element discretisations of partial differential equations (PDEs) is vast. (Among the most efficient ones for finite element systems on unstructured meshes are the newly developed versions of multi-grid methods (cf. [16], [8], [28], [3], [19], [4], [12]) or the \mathcal{H} -matrices (cf. [13], [14], [15])).

The new solution concept for lattice equations which we will introduce in this paper is as follows. For the given (discrete) lattice equation, we will derive a continuous partial differential equation (PDE) and a corresponding prolongation which maps discrete grid functions to continuous finite element functions. Such a prolongation allows to use the finite element discretisation of the associated PDE as a preconditioner for the lattice equation and fast solvers (e.g., multigrid methods) are available for the efficient realisation of this preconditioner.

Our *concept* (which we will denote as the *recovery method*) of transferring the discrete lattice equation to a finite element discretisation of a continuous PDE is quite general. In this paper, we will introduce the abstract concept along with the simple linear, scalar model problem of heat conduction through a lattice. However, we emphasize that the concept of the recovery method is by no means limited to this model problem. Forthcoming papers will address the application to larger problem classes such as vector-valued problems, indefinite problems, and parameter-dependent or singularly perturbed problems.

Various averaging and agglomeration techniques for extracting coarser systems from finite element stiffness matrices exist in the literature in the context, e.g., of multi-grid methods. In contrast to these approaches, the lattices which will be considered here may have a much more complicated geometric structure compared to lattices which are the set of edges of finite element meshes. Furthermore, the theory which will be developed in this paper allows to predict, from simple geometric quantities which can be computed in a preprocessing phase, the performance of the recovery method to avoid the failure of the solution procedure. The underlying idea of our approach is to match local energies in the lattices with local energies in finite element meshes. In the context of discrete homogenisation, an alternative approach which was based on averaged Taylor expansions has been presented (cf. [16, Sec. 7]).

Our approach is an alternative to the *algebraic multi-grid methods* (see, e.g., [20], [25]) which can be applied to discrete lattice equations as well. We do not elaborate a comparison of the recovery method with the algebraic multigrid method but focus here on the presentation of the fundamental concepts of the recovery method.

The paper is structured as follows.

In Section 2, we will introduce the problem of heat conduction in lattice materials as our model problem for the development of the concept of the recovery method.

In Section 3, the recovery method will be presented which consists of the following steps: First, a domain along with a finite element mesh is constructed where the

nodal points of the mesh coincide with the nodes in the lattice. In the second step, a (discrete) bilinear form is constructed on the lattice defined by the edges of the finite element mesh. This bilinear form will have equivalent energy as the given bilinear form of the original lattice equation. In the third step, a bilinear form on the continuous level is constructed which, again, has equivalent energy as the original lattice system.

In Section 4 we will prove that the linear system which corresponds to the continuous bilinear form serves as an quasi-optimal preconditioner for the original lattice equation. Hence, standard solvers for linear finite element systems can be employed to realise the application of the preconditioner.

In Section 5, we will develop the recovery method for problems with Dirichlet-type constraints. More precisely, we will consider the problem where the values of the solution of the lattice equations is prescribed in a subset of the lattice points.

2 Model Problem

In this section, we will formulate the model problem and introduce the relevant notations.

Let $\Theta := \{x_1, x_2, \dots, x_N\} \subset \mathbb{R}^d$ denote the set of nodal points and let $\mathcal{E} \subset \Theta \times \Theta$ be a symmetric set of edges, i.e., $e = (x, y) \in \mathcal{E}$ implies $(y, x) \in \mathcal{E}$. The set of nodal points together with the set of edges \mathcal{E} form the graph \mathcal{G} of the lattice.

From the physical point of view, we shall deal with equations on the lattice \mathcal{G} which are of the same (abstract) form as the equations of linear heat flow, i.e., are described by scalar discrete potential equations of second order. First, we will consider the case that no essential constraints at the nodes are described. The case of essential constraints will be treated in Section 5.

The heat conductivity through an edge $(x, y) \in \mathcal{E}$ is described by a symmetric, positive mapping $\mathbf{a} = (a_e)_{e \in \mathcal{E}}$ with

$$\left. \begin{array}{l} a_{(x,y)} = a_{(y,x)} \\ a_{(x,y)} > 0 \end{array} \right\} \quad \forall (x, y) \in \mathcal{E}.$$

Let S denote the space of (unconstrained) grid functions

$$S := \mathbb{R}^\Theta := \{\mathbf{u} \mid \mathbf{u} : \Theta \rightarrow \mathbb{R}\}.$$

The quotient space S/\mathbb{R} where the equivalence classes are formed by functions which differ only by a constant grid function will be employed for the following Laplace-type problem:

Let $F \in (S/\mathbb{R})'$ be given. Find $\mathbf{u} = (u_x)_{x \in \Theta} \in S/\mathbb{R}$ so that

$$\mathbf{B}(\mathbf{u}, \mathbf{v}) := \frac{1}{2} \sum_{e=(x,y) \in \mathcal{E}} \frac{a_e}{h_e} (u_y - u_x) (v_y - v_x) = F(\mathbf{v}) \quad \forall \mathbf{v} = (v_x)_{x \in \Theta} \in S/\mathbb{R}, \quad (2.1)$$

where $h_e := \|x - y\|$.

This equation has a unique solution as can be seen from the following well-known theorem.

Theorem 2.1 *Let the lattice be connected. The variational problem (2.1) has a unique solution $u \in S/\mathbb{R}$ for any right-hand side $F \in (S/\mathbb{R})'$.*

Proposition 2.2 *Let the lattice be connected. Then, $F \in (S/\mathbb{R})'$ is equivalent to $F \in S'$ and $F(\mathbf{1}) = 0$, where $\mathbf{1} : \Theta \rightarrow \mathbb{R}$ is the function with constant value 1.*

The variational problem (2.1) can be interpreted as a system of finite difference equations. We are testing equation (2.1) for all $z \in \Theta$ with the unit vectors $\mathbf{e}_z = (e_{z,x})_{x \in \Theta} \in S$, where

$$e_{z,x} := \begin{cases} 1 & x = z, \\ 0 & x \in \Theta \setminus \{z\}. \end{cases}$$

For $z \in \Theta$, we obtain the relation

$$\frac{1}{2} \sum_{e=(x,y) \in \mathcal{E}} \frac{a_e}{h_e} (u_y - u_x) (e_{z,y} - e_{z,x}) = \frac{1}{2} \sum_{\substack{x \in \Theta: \\ e=(z,x) \in \mathcal{E}}} \frac{a_e}{h_e} (u_z - u_x).$$

By setting $F_z := F(\mathbf{e}_z)$ and

$$A_{xy} := \begin{cases} \sum_{\substack{z \in \Theta: \\ e=(x,z) \in \mathcal{E}}} a_e/h_e & \text{if } x = y, \\ -a_e/h_e & \text{if } e \in \mathcal{E}, \\ 0 & \text{otherwise,} \end{cases}$$

we obtain the finite difference equations

$$\sum_{y \in \Theta} A_{xy} u_y = F_x \quad \forall x \in \Theta,$$

and use the short notation $\mathbf{A}\mathbf{u} = \mathbf{F}$. To get an equivalent system to the variational formulation (2.1), we have to restrict the right-hand side and the solution in (2.2) to appropriate quotient spaces: For given $\mathbf{F} \in (S/\mathbb{R})'$, find $\mathbf{u} \in S/\mathbb{R}$ such that

$$\mathbf{A}\mathbf{u} = \mathbf{F}. \tag{2.2}$$

3 The Recovery Method

In this section, we will introduce the recovery method for transferring given lattice equations into a continuous partial differential equation for which efficient solvers are available. This efficient solver then serves, via the recovery method, as a preconditioner for the given lattice equation. In this paper, we introduce the recovery method for the simple model problem of heat conduction which was introduced in the previous section.

The idea is to define a bilinear form for (continuous) finite element functions which has in a certain sense equivalent energy. The construction consists of the definition of a domain $\Omega \subset \mathbb{R}^d$ for the continuous problem and the definition of the coefficient function in the partial differential equation.

We begin with the definition of the domain Ω . For a subset $M \subset \mathbb{R}^d$, we write $\text{int}(M)$ for the interior of M .

Theorem 3.1 *Let $\Theta \subset \mathbb{R}^d$, $d \in \{2, 3\}$, denote a discrete set of points with $\text{card } \Theta \geq d+1$. Then, the Voronoï method defines a triangulation \mathcal{G}_{FE} of d -dimensional, disjoint simplices where the set of mesh points Θ_{FE} satisfies $\Theta_{FE} = \Theta$. For non-identical elements $\tau, t \in \mathcal{G}_{FE}$, the intersection $\tau \cap t$ is either empty, a common point, a common edge, or -for $d = 3$ - a common face.*

The mesh \mathcal{G}_{FE} covers the set

$$\Omega := \text{int} \overline{\bigcup_{\tau \in \mathcal{G}_{FE}} \tau}.$$

Remark 3.2 *An algorithm for assembling a triangulation (Delaunay triangulation) as in Theorem 3.1 is described, e.g., in [9], [26], [27], [5].*

Assumption 3.3 *The set $\Omega \subset \mathbb{R}^d$ is a polygonal (polyhedral for $d = 3$) Lipschitz domain.*

Note that in three space dimensions not every polyhedral domain is Lipschitz.

The existence of the triangulation \mathcal{G}_{FE} does **not** ensure that the parameters which are measuring the quality of the triangles, e.g., the maximal/minimal angle or the maximal ratio of diameters of neighbouring elements, is moderately bounded. In this light, we will introduce some mesh-dependent parameters which may serve as indicators for the performance of the recovery method.

Definition 3.4 *The constant C_{sr} measures the shape regularity of the mesh \mathcal{G}_{FE}*

$$C_{sr} := \max_{\tau \in \mathcal{G}_{FE}} \frac{h_\tau}{\rho_\tau}, \quad (3.1)$$

where $h_\tau := \text{diam } \tau$ and ρ_τ is the radius of the largest inscribed ball in τ .

We make an assumption on the “compatibility” of the meshes and introduce some notation.

Let the edges in \mathcal{G}_{FE} be denoted by \mathcal{E}_{FE} . To distinguish in the notation the edges in \mathcal{E}_{FE} from edges in the given lattice \mathcal{E} we will use a tilde superscript for edges in \mathcal{E}_{FE} . For $\tilde{e} = (x, y) \in \mathcal{E}_{FE}$, we have $x, y \in \Theta$ and we may associate with \tilde{e} a minimal path, i.e., a path with a minimal number of segments, $\pi(\tilde{e}) = (e_1, e_2, \dots, e_{q(\tilde{e})}) \subset \mathcal{E}$ such that

$$x_0 = x, \quad x_{q(e)} = y \quad \text{and} \quad e_i = (x_{i-1}, x_i), \quad 1 \leq i \leq q(\tilde{e}).$$

connecting x and y . In an analogous way, we associate such a path $\pi_{FE}(e) \subset \mathcal{E}_{FE}$ for each $e \in \mathcal{E}$.

Assumption 3.5 *The lattice \mathcal{G} and the mesh \mathcal{G}_{FE} are connected.*

Remark 3.6 *The connectivity of the lattice \mathcal{G} and the connectivity of the mesh \mathcal{G}_{FE} imply that $\pi(\tilde{e}) \neq \emptyset$ for every $\tilde{e} \in \mathcal{E}_{FE}$ and $\pi_{FE}(e) \neq \emptyset$ for every $e \in \mathcal{E}$.*

Assumption 3.7 (a) *There exists a constant $\eta > 0$ such that,*

1. *for every $\tilde{e} = (x, y) \in \mathcal{E}_{FE}$, we have*

$$\|z_2 - z_1\| \leq \eta \|x - y\|, \quad (z_1, z_2) \in \pi(\tilde{e}),$$

where $\|\cdot\|$ denotes the Euclidean length of a vector,

2. *for every $e = (x, y) \in \mathcal{E}$, we have*

$$\|z_2 - z_1\| \leq \eta \|x - y\|, \quad (z_1, z_2) \in \pi_{FE}(e).$$

(b) *There exists $\bar{n} < \infty$ such that,*

1. *for every $(x, y) \in \mathcal{E}$, we have*

$$\text{card} \{ \tilde{e} \in \mathcal{E}_{FE} : (x, y) \in \pi(\tilde{e}) \} \leq \bar{n}$$

2. *for every $(x, y) \in \mathcal{E}_{FE}$, we have*

$$\text{card} \{ e \in \mathcal{E} : (x, y) \in \pi_{FE}(e) \} \leq \bar{n}.$$

(c) *There exists $\bar{q} < \infty$ such that*

$$\max \left\{ \sup_{e \in \mathcal{E}} \text{card} \pi_{FE}(e), \sup_{\tilde{e} \in \mathcal{E}_{FE}} \text{card} \pi(\tilde{e}) \right\} \leq \bar{q}.$$

Our goal is to replace the lattice equations (2.1) by a finite element discretisation of a Poisson equation on the mesh \mathcal{G}_{FE} . This is done in two steps.

(a) Define a system of lattice equations on the edges \mathcal{E}_{FE} of \mathcal{G}_{FE} which has equivalent energy.

(b) Replace the lattice equations on \mathcal{E}_{FE} by an averaged Poisson problem on Ω .

3.1 Definition of a system of lattice equations on \mathcal{E}_{FE} with equivalent energy

In this section, we will introduce a system of lattice equations on the set of finite element edges which has equivalent energy as the original equations. Our approach is based on a suitable local average of the conductivity coefficients $(a_e)_{e \in \mathcal{E}}$ along the paths $\pi(e)$. In this light, we will introduce some notations.

Notation 3.8 For $\tilde{e} = (x, y) \in \mathcal{E}_{FE}$, let

$$a_{\tilde{e}}^{FE} := \min_{e \in \pi(\tilde{e})} a_e, \quad A_{\tilde{e}}^{FE} := \max_{e \in \pi(\tilde{e})} a_e,$$

$$\bar{a}_{\tilde{e}}^{FE} := \sqrt{A_{\tilde{e}}^{FE} a_{\tilde{e}}^{FE}}, \quad \rho := \max_{e \in \mathcal{E}} \max_{\tilde{e} \in \mathcal{E}_{FE}: e \in \pi(\tilde{e})} \sqrt{A_{\tilde{e}}^{FE} / a_{\tilde{e}}^{FE}}.$$

We introduce the bilinear form

$$\mathbf{B}_{FE}(\mathbf{u}, \mathbf{v}) := \frac{1}{2} \sum_{(x,y) \in \mathcal{E}_{FE}} \bar{a}_{(x,y)}^{FE} \frac{(u_y - u_x)(v_y - v_x)}{\|x - y\|}. \quad (3.2)$$

Theorem 3.9 Let Assumptions 3.5 and 3.7 be satisfied. The bilinear forms \mathbf{B}_{FE} and \mathbf{B} define equivalent energies:

$$\frac{1}{\eta \bar{q} \bar{n} \rho} \mathbf{B}(\mathbf{u}, \mathbf{u}) \leq \mathbf{B}_{FE}(\mathbf{u}, \mathbf{u}) \leq \eta \bar{q} \bar{n} \rho \mathbf{B}(\mathbf{u}, \mathbf{u}) \quad \forall \mathbf{u} \in \mathbb{R}^\Theta. \quad (3.3)$$

Proof. First, we will consider the right inequality in (3.3).

For $\tilde{e} = (x, y) \in \mathcal{E}_{FE}$, we get with $q = \text{card } \pi(\tilde{e})$

$$\begin{aligned} \frac{(u_x - u_y)^2}{\|x - y\|} &\leq q \sum_{e=(z_1, z_2) \in \pi(\tilde{e})} \frac{(u_{z_2} - u_{z_1})^2}{h_{\tilde{e}}} \leq \eta q \sum_{e=(z_1, z_2) \in \pi(\tilde{e})} \frac{(u_{z_2} - u_{z_1})^2}{h_e} \\ &\leq \frac{\eta q}{a_{\tilde{e}}^{FE}} \sum_{e=(z_1, z_2) \in \pi(\tilde{e})} \frac{a_e (u_{z_2} - u_{z_1})^2}{h_e} \end{aligned}$$

and, hence,

$$\begin{aligned} \mathbf{B}_{FE}(\mathbf{u}, \mathbf{u}) &= \frac{1}{2} \sum_{(x,y) \in \mathcal{E}_{FE}} \bar{a}_{(x,y)}^{FE} \frac{(u_y - u_x)^2}{\|x - y\|} \leq \eta \bar{q} \frac{1}{2} \sum_{\tilde{e} \in \mathcal{E}_{FE}} \frac{\bar{a}_{\tilde{e}}^{FE}}{a_{\tilde{e}}^{FE}} \sum_{(x,y) \in \pi(\tilde{e})} \frac{a_{(x,y)} (u_y - u_x)^2}{\|y - x\|} \\ &= \eta \bar{q} \frac{1}{2} \sum_{e=(x,y) \in \mathcal{E}} \frac{a_{(x,y)} (u_y - u_x)^2}{\|y - x\|} \sum_{\tilde{e} \in \mathcal{E}_{FE}: (x,y) \in \pi(\tilde{e})} \bar{a}_{\tilde{e}}^{FE} / a_{\tilde{e}}^{FE} \\ &\leq \eta \bar{q} \bar{n} \rho \mathbf{B}(\mathbf{u}, \mathbf{u}). \end{aligned}$$

The opposite estimate is derived by interchanging the roles of \mathcal{G}_{FE} and \mathcal{G} . ■

Remark 3.10 (a) In the special case $\mathcal{E}_{FE} = \mathcal{E}$, we may choose $\pi(e) = \pi_{FE}(e) = e$. Hence, all constants $\eta, \bar{q}, \bar{n}, \rho$ in (3.3) equal one and the bilinear forms \mathbf{B}_{FE} and \mathbf{B} coincide.

(b) Note that the constant ρ in (3.3) is moderately bounded also for conductivity coefficients with large global ratio $\max_{e \in \mathcal{E}} a_e / \min_{e \in \mathcal{E}} a_e$ as long as the local variations (measured by $\max_{\tilde{e} \in \mathcal{E}_{FE}: e \in \pi(\tilde{e})} \sqrt{A_{\tilde{e}}^{FE} / a_{\tilde{e}}^{FE}}$) are moderately bounded.

3.2 Recovery of the continuous variational form

In this step, we will define, for the given system of lattice equations, a bilinear form on the continuous level along with a transfer mapping which has equivalent energy.

We start with some preliminaries on local finite element matrices and associated finite difference operators.

Consider a simplex $\tau = \text{conv}\{\mathbf{x}_1, \dots, \mathbf{x}_{d+1}\} \in \mathcal{G}_{FE}$ and denote by b_i , $1 \leq i \leq d+1$, the corresponding local affine Lagrange basis (“hat functions”) on τ . The local finite element matrix $\mathbf{L}_\tau = (L_{i,j})_{i,j=1}^{d+1}$ is defined by

$$L_{i,j} := \int_{\tau} \langle \nabla b_i, \nabla b_j \rangle d\mathbf{x}, \quad 1 \leq i, j \leq d+1.$$

Let $\mathbf{u} = (u_i)_{i=1}^{d+1} \in \mathbb{R}^{d+1}$ be a grid function with values u_i at \mathbf{x}_i , $1 \leq i \leq d+1$. For simplicity, we set $\mathbf{x}_{d+2} := \mathbf{x}_1$ and $\mathbf{x}_0 := \mathbf{x}_{d+1}$ and use this convention also for \mathbf{u} and \mathbf{v} .

Lemma 3.11 *There exist constants $0 < c_2, C_2 < \infty$ depending only on the constant C_{sr} in (3.1) and the dimension d such that*

$$c_2 \sum_{i=1}^{d+1} (u_{i+1} - u_{i-1})^2 \leq h_\tau^{2-d} \mathbf{u}^\top \mathbf{L}_\tau \mathbf{u} \leq C_2 \sum_{i=1}^{d+1} (u_{i+1} - u_{i-1})^2. \quad (3.4)$$

Proof. We will work out the proof only in the case $d = 2$ and choose a counter-clockwise numbering of the vertices of τ .

We obtain by using $\mathbf{e}_i := \mathbf{x}_{i+1} - \mathbf{x}_{i-1}$, $\mathbf{v}^\perp = (v_2, -v_1)^\top$, and $|\tau| = \text{area}(\tau)$ the representations

$$\nabla b_i = \frac{(\mathbf{x}_{i+1} - \mathbf{x}_{i-1})^\perp}{2|\tau|} \quad \text{and} \quad \mathbf{L}_\tau = \frac{1}{4|\tau|} \begin{bmatrix} \|\mathbf{e}_1\|^2 & \langle \mathbf{e}_1, \mathbf{e}_2 \rangle & \langle \mathbf{e}_1, \mathbf{e}_3 \rangle \\ \langle \mathbf{e}_1, \mathbf{e}_2 \rangle & \|\mathbf{e}_2\|^2 & \langle \mathbf{e}_2, \mathbf{e}_3 \rangle \\ \langle \mathbf{e}_1, \mathbf{e}_3 \rangle & \langle \mathbf{e}_2, \mathbf{e}_3 \rangle & \|\mathbf{e}_3\|^2 \end{bmatrix}.$$

Hence,

$$\begin{aligned}
\mathbf{u}^\top \mathbf{L}_\tau \mathbf{v} &= \sum_{i=1}^3 u_i \sum_{j=1}^3 \frac{\langle \mathbf{e}_i, \mathbf{e}_j \rangle}{4|\tau|} v_j = \frac{1}{4|\tau|} \left\langle \sum_{i=1}^3 u_i \mathbf{e}_i, \sum_{j=1}^3 v_j \mathbf{e}_j \right\rangle \\
&= \frac{1}{4|\tau|} \langle (u_3 - u_1) \mathbf{e}_3 + (u_2 - u_1) \mathbf{e}_2, (v_3 - v_1) \mathbf{e}_3 + (v_2 - v_1) \mathbf{e}_2 \rangle \\
&= \frac{1}{4|\tau|} \begin{pmatrix} u_1 - u_3 \\ u_2 - u_1 \end{pmatrix}^\top \begin{bmatrix} \|\mathbf{e}_3\|^2 & -\langle \mathbf{e}_3, \mathbf{e}_2 \rangle \\ -\langle \mathbf{e}_3, \mathbf{e}_2 \rangle & \|\mathbf{e}_2\|^2 \end{bmatrix} \begin{pmatrix} v_1 - v_3 \\ v_2 - v_1 \end{pmatrix} \\
&=: \begin{pmatrix} u_1 - u_3 \\ u_2 - u_1 \end{pmatrix}^\top \tilde{\mathbf{L}}_\tau \begin{pmatrix} v_1 - v_3 \\ v_2 - v_1 \end{pmatrix}.
\end{aligned}$$

The eigenvalues λ_1, λ_2 of $\tilde{\mathbf{L}}_\tau$ can be estimated by

$$c_1 := \frac{\min \{ \|\mathbf{e}_3\|^2, \|\mathbf{e}_2\|^2 \}}{4|\tau|} \leq \lambda_1, \lambda_2 \leq \frac{\|\mathbf{e}_3\|^2 + \|\mathbf{e}_2\|^2}{4|\tau|} =: C_1.$$

The constants c_1, C_1 are positive depending only on the constant C_{sr} as in (3.1) and, in general, on the space dimension d . Thus,

$$c_1 ((u_1 - u_3)^2 + (u_2 - u_1)^2) \leq \mathbf{u}^\top \mathbf{L}_\tau \mathbf{u} \leq C_1 ((u_1 - u_3)^2 + (u_2 - u_1)^2).$$

■

We will use Lemma 3.11 to associate, for every triangle $\tau \in \mathcal{G}_{FE}$, a *local* bilinear form which has an equivalent energy as the *restriction* of the global bilinear form \mathbf{B}_{FE} to the edges of τ .

The restricted bilinear form is defined by

$$\mathbf{B}_{FE}^\tau(\mathbf{u}, \mathbf{v}) := \frac{1}{2} \sum_{i=1}^{d+1} \bar{a}_{\mathbf{e}_i}^{FE} \frac{(u_{i+1} - u_{i-1})(v_{i+1} - v_i)}{h_i},$$

where $\mathbf{e}_i := \mathbf{x}_{i+1} - \mathbf{x}_{i-1}$ is a simplex edge as in the proof of Lemma 3.11 and $h_i := \|\mathbf{e}_i\|$. Let us introduce the constants and averages

$$\begin{aligned}
a_\tau^{FE} &:= \min_{1 \leq i \leq d} \bar{a}_{\mathbf{e}_i}^{FE} & A_\tau^{FE} &:= \max_{1 \leq i \leq d} \bar{a}_{\mathbf{e}_i}^{FE} \\
\bar{a}_\tau^{FE} &:= \sqrt{a_\tau^{FE} A_\tau^{FE}} & \lambda &:= \max_{\tau \in \mathcal{G}_{FE}} \sqrt{A_\tau^{FE} / a_\tau^{FE}}
\end{aligned}$$

and the local bilinear form

$$B^\tau(u, v) := \bar{a}_\tau^{FE} h_\tau^{1-d} \int_\tau \langle \nabla u, \nabla v \rangle dx \quad \forall u, v \in \mathbb{P}_1.$$

Lemma 3.12 *Let $\tau \in \mathcal{G}_{FE}$ be a simplex with vertices $(\mathbf{x}_i)_{i=1}^{d+1}$. For $u \in \mathbb{P}_1$, let $\mathbf{u} = (u_i)_{i=1}^d$ denote the nodal values of u at \mathbf{x}_i , $1 \leq i \leq d+1$. Then,*

$$c_3 \lambda^{-1} \mathbf{B}_{FE}^\tau(\mathbf{u}, \mathbf{v}) \leq B^\tau(u, v) \leq C_3 \lambda \mathbf{B}_{FE}^\tau(\mathbf{u}, \mathbf{v}) \quad \forall u, v \in \mathbb{P}_1,$$

where c_3, C_3 are positive constants depending only on the constant C_{sr} in (3.1) and the dimension d .

Proof. Lemma 3.11 along with the definition of the averaged coefficient \bar{a}_τ^{FE} imply

$$\frac{c_2}{\lambda} \sum_{i=1}^{d+1} \bar{a}_{\mathbf{e}_i}^{FE} (u_{i+1} - u_{i-1})^2 \leq \bar{a}_\tau^{FE} h_\tau^{2-d} \mathbf{u}^\top \mathbf{L}_\tau \mathbf{u} \leq C_2 \lambda \sum_{i=1}^{d+1} \bar{a}_{\mathbf{e}_i}^{FE} (u_{i+1} - u_{i-1})^2$$

with c_2, C_2 as in (3.11). The estimate $ch_\tau \leq h_i \leq h_\tau$ is valid with a constant c depending only on C_{sr} (cf. (3.1)) leading to the proof of the assertion. ■

By summing over all local bilinear forms B^τ we derive the global variational formulation as follows.

Define the coefficient function $a : \Omega \rightarrow \mathbb{R}$ by

$$a|_\tau := \bar{a}_\tau^{FE} h_\tau^{1-d}. \quad (3.5)$$

The finite element space of continuous piecewise linear functions on \mathcal{G}_{FE} is denoted by

$$V^{FE} := \{u \in C^0(\bar{\Omega}) \mid \forall \tau \in \mathcal{G}_{FE} : u|_\tau \in \mathbb{P}_1\}. \quad (3.6)$$

The standard local nodal basis is denoted by $(b_x)_{x \in \Theta}$. The finite element interpolation operator on \mathcal{G}_{FE} is denoted by $I_{FE}^{int} : \mathbb{R}^\Theta \rightarrow V^{FE}$:

$$(I_{FE}^{int} \mathbf{u})(x) = \sum_{y \in \Theta} u_y b_y(x).$$

For $u, v \in V^{FE}$, the global bilinear form which is associated to the lattice equations is defined by

$$B(u, v) := \int_\Omega a(x) \langle \nabla u, \nabla v \rangle dx. \quad (3.7)$$

We will prove next that this bilinear form has the same energy as the original lattice.

Theorem 3.13 *Let Assumptions 3.3 and 3.5 be satisfied. For all $\mathbf{u}, \mathbf{v} \in \mathbb{R}^\Theta$ and $u := I_{FE}^{int} \mathbf{u}$, $v := I_{FE}^{int} \mathbf{v}$ we have*

$$c_5 \mathbf{B}_{FE}(\mathbf{u}, \mathbf{v}) \leq B(u, v) \leq C_5 \mathbf{B}_{FE}(\mathbf{u}, \mathbf{v})$$

with

$$c_5 := \frac{c_4}{\eta \bar{q} \bar{n} \rho \lambda} \quad \text{and} \quad C_5 := C_4 \lambda \eta \bar{q} \bar{n} \rho.$$

The positive constants c_4, C_4 only depend on C_{sr} (cf. (3.1)) and the dimension d .

Proof. The result for the bilinear form B instead of B^τ simply follows by summing over (3.4). ■

If the ratio of the global bounds of the coefficient function a are moderately bounded over the domain it is reasonable to introduce the global average

$$\begin{aligned} a_{\max} &:= \max \{a|_\tau : \tau \in \mathcal{G}_{FE}\} & a_{\min} &:= \min \{a|_\tau : \tau \in \mathcal{G}_{FE}\} \\ \bar{a} &:= \sqrt{a_{\min} a_{\max}} & \mu &:= \sqrt{a_{\max}/a_{\min}} \end{aligned} \tag{3.8}$$

and the bilinear form $\overline{B}(\cdot, \cdot)$ with constant coefficient

$$\overline{B}(u, v) = \bar{a} \int_{\Omega} \langle \nabla u, \nabla v \rangle dx.$$

In the energy estimate, the factor μ has to be introduced.

Corollary 3.14 *Let Assumptions 3.3, 3.5 be satisfied. For all $\mathbf{u}, \mathbf{v} \in \mathbb{R}^\Theta$ and $u := I_{FE}^{int} \mathbf{u}$, $v := I_{FE}^{int} \mathbf{v}$ we have*

$$\frac{c_5}{\mu} \mathbf{B}_{FE}(\mathbf{u}, \mathbf{v}) \leq B(u, v) \leq C_5 \mu \mathbf{B}_{FE}(\mathbf{u}, \mathbf{v})$$

with c_5, C_5 as in Theorem 3.13.

Corollary 3.15 *Theorem 3.13 shows that the ellipticity of the continuous bilinear form $B(\cdot, \cdot)$ (w.r.t. the quotient space V^{FE}/\mathbb{R} (cf. (3.6)) carries over to the bilinear form $\mathbf{B}(\cdot, \cdot)$.*

4 A Finite Element Preconditioner based on the Recovery Method

In the previous section, we have introduced the recovery method which associates a variational formulation on the continuous level to the given lattice equations along with a transfer mapping between discrete grid functions and finite element functions.

In this section, we will show that the stiffness matrix \mathbf{A}_{FE} which corresponds to the finite element discretisation of $B(\cdot, \cdot)$ on the mesh \mathcal{G}_{FE} provides a quasi-optimal preconditioner of the system of lattice equations (2.2).

The preconditioned system takes the form

$$\mathbf{A}_{FE}^{-1} \mathbf{A} \mathbf{u} = \mathbf{A}_{FE}^{-1} \mathbf{F}.$$

Recall that the matrix \mathbf{A} is regular on the subspace S/\mathbb{R} and we understand \mathbf{A}_{FE}^{-1} as a mapping $\mathbf{A}_{FE}^{-1} : (S/\mathbb{R})' \rightarrow (S/\mathbb{R})$.

The Richardson iteration for the preconditioned system is given by

$$\mathbf{u}^{(i+1)} := \mathbf{u}^{(i)} - \alpha \mathbf{A}_{FE}^{-1} (\mathbf{A} \mathbf{u}^{(i)} - \mathbf{F})$$

with some damping parameter α . The error $\mathbf{e}^{(i)} := \mathbf{u}^{(i)} - \mathbf{u}$ satisfies the equation

$$\mathbf{e}^{(i+1)} := (\mathbf{I} - \alpha \mathbf{A}_{FE}^{-1} \mathbf{A}) \mathbf{e}^{(i)}$$

and we will prove in Theorem 4.1 that the error converges exponentially with respect to the energy norm, i.e.,

$$\|\mathbf{I} - \alpha \mathbf{A}_{FE}^{-1} \mathbf{A}\|_{\mathbf{A}_{FE}} < c_0 < 1.$$

For a vector $\mathbf{x} \in \mathbb{R}^\Theta$, the norm $\|\cdot\|_{\mathbf{A}_{FE}}$ is

$$\|\mathbf{x}\|_{\mathbf{A}_{FE}} := (\mathbf{x}^\top \mathbf{A}_{FE} \mathbf{x})^{1/2}$$

and, for a grid operator $\mathbf{M} \in \mathbb{R}^{\Theta \times \Theta}$, $\|\mathbf{M}\|_{\mathbf{A}_{FE}}$ denotes the corresponding operator norm. The Euclidean norm is denoted by $\|\cdot\|$.

Theorem 4.1 *Let Assumptions 3.3 and 3.5 be satisfied. Let $\alpha = \frac{2}{C_5^{-1} + c_5^{-1}}$ with C_5, c_5 as in Theorem 3.13. Then*

$$\|\mathbf{I} - \alpha \mathbf{A}_{FE}^{-1} \mathbf{A}\|_{\mathbf{A}_{FE}} \leq \frac{C_5 - c_5}{C_5 + c_5}.$$

Proof. Let $\|\cdot\|$ denote the standard Euclidean norm in \mathbb{R}^Θ . We have

$$\begin{aligned} \|\mathbf{I} - \alpha \mathbf{A}_{FE}^{-1} \mathbf{A}\|_{\mathbf{A}_{FE}} &= \sup_{\mathbf{x} \in \mathbb{R}^\Theta \setminus \{0\}} \frac{\|\mathbf{x} - \alpha \mathbf{A}_{FE}^{-1} \mathbf{A} \mathbf{x}\|_{\mathbf{A}_{FE}}}{\|\mathbf{x}\|_{\mathbf{A}_{FE}}} = \sup_{\mathbf{y} \in \mathbb{R}^\Theta \setminus \{0\}} \frac{\|\mathbf{y} - \alpha \mathbf{A}_{FE}^{-1/2} \mathbf{A} \mathbf{A}_{FE}^{-1/2} \mathbf{y}\|}{\|\mathbf{y}\|} \\ &= \max \left\{ |\lambda| : \lambda \text{ is an eigenvalue of } \mathbf{I} - \alpha \mathbf{A}_{FE}^{-1/2} \mathbf{A} \mathbf{A}_{FE}^{-1/2} \right\}. \end{aligned}$$

Theorem 3.13 implies that

$$\frac{1}{C_5} \leq \|\mathbf{A}_{FE}^{-1/2} \mathbf{A} \mathbf{A}_{FE}^{-1/2}\| \leq \frac{1}{c_5}.$$

Thus, by choosing $\alpha = \frac{2}{C_5^{-1} + c_5^{-1}}$, we obtain

$$\|\mathbf{I} - \alpha \mathbf{A}_{FE}^{-1} \mathbf{A}\|_{\mathbf{A}_{FE}} \leq \frac{C_5 - c_5}{C_5 + c_5}.$$

■

Thus, we have transferred the lattice equation to a bilinear form $B(\cdot, \cdot)$ such that its finite element discretisation leads to a system matrix \mathbf{A}_{FE} which serves as an quasi-optimal preconditioner. We have traced explicitly the dependence of the bounds which describe the equivalence of energy on

- the compatibility of the finite element mesh with the given lattice, (cf. (3.7)),
- the shape regularity of the finite element mesh (cf. (3.1)),
- the *local* variations of the conductivity coefficients (cf. Notation 3.8, (3.8)).

Since these constants can be computed easily in a preprocessing phase of the computations, the method allows to predict the efficiency of the recovery algorithm in advance.

Note that the system \mathbf{A}_{FE} has the same dimension as the original system \mathbf{A} . Since \mathbf{A}_{FE} corresponds to the variational form $B(\cdot, \cdot)$ on the continuous level, a vast supply of efficient solvers for the preconditioner \mathbf{A}_{FE} exists in the literature. The most efficient solvers for systems of linear equations are multi-grid methods. In the recent years, various multi-grid solvers have been developed for solving elliptic boundary value problems on *unstructured* meshes.

Since the main objective of this paper is the introduction of the recovery method for the transfer of unstructured discrete lattice equations to variational forms, we will not present in detail linear solvers for the preconditioner. In [16], [8], [28], [3], [19], [4], [20], [12], [25] various variants of multi-grid methods are described for solving elliptic problems on unstructured meshes and/or discontinuous coefficients.

5 Dirichlet-type constraints

In this section, we will consider the problem where the values of the solution have prescribed value zero on a subset Θ_0 with $\emptyset \neq \Theta_0 \subsetneq \Theta$.

In this case, the space of grid functions is given by

$$S_0 := \{ \mathbf{u} \in \mathbb{R}^\Theta \mid \forall x \in \Theta_0 : \mathbf{u}(x) = 0 \}.$$

The recovery method for the derivation of the bilinear form $B(u, v)$ is applied verbatim as for the unconstrained problem (2.1) and the definition (3.5), (3.7) is used without changes. However, the finite element space V^{FE} (cf. (3.6)) has to take into account the essential constraints and we set

$$V_0^{FE} := \{ u \in V^{FE} \mid \forall x \in S_0 : u(x) = 0 \}. \quad (5.1)$$

Remark 5.1 (a) Note that the evaluation of functions $u \in H^1(\Omega)$ at discrete points $x \in \Omega$ is not defined since $H^1(\Omega) \not\subset C^0(\Omega)$. However, for finite element functions $u \in V^{FE}$, the point evaluation is well defined.

(b) The recovery method can be interpreted as the inverse of the transfer “boundary value problem and basis of the finite element space \rightarrow stiffness matrix” in the following sense. Consider the special case $\mathcal{G} = \mathcal{G}_{FE}$, where \mathcal{G}_{FE} is a triangulation of a domain Ω with boundary Γ . Assume the lattice equations originates from the finite element

discretisation of the continuous Laplace problem with homogeneous Dirichlet boundary conditions at Γ on the mesh \mathcal{G}_{FE} . Then, the usual finite element space on \mathcal{G}_{FE} for the Dirichlet problem coincides with the recovered space V_0^{FE} as in (5.1).

The proof that the bilinear form for the lattice equation and the bilinear form on the continuous level have equivalent energies is a repetition of the proof of Theorem 3.13. The constants of equivalency are the same as in Theorem 3.13.

Similarly, Theorem 4.1 holds verbatim for the problem with Dirichlet constraints.

Acknowledgement: This work was supported by the Army Research Office Grant DAAD19-99-0149 and by the National Science Foundation Grant DMS-9802367. The second author was supported by the Swiss Federal Office for Education and Science, Grant 01-0025-1/2 (as a part of the HMS 2000-Research Training Network “Homogenization and Multiple Scales” of the European Union) and by the Swiss National Science Foundation, Grant 21-58891.99.

References

- [1] I. Babuška and B. Guo. Problems of unbounded lattices, mathematical framework. *to appear*.
- [2] I. Babuška and S. Sauter. Algebraic Algorithms for the Analysis of Mechanical Trusses. Technical Report 16-2002, Universität Zürich, <http://www.math.unizh.ch/fileadmin/math/preprints/16-02.pdf>, 2002.
- [3] R. E. Bank and J. Xu. A Hierarchical Basis Multi-Grid Method for Unstructured Grids. In W. Hackbusch and G. Wittum, editors, *Fast Solvers for Flow Problems, Proceedings of the Tenth GAMM-Seminar, Kiel*. Verlag Vieweg, 1995.
- [4] T. Chan, J. Xu, and L. Zikatanov. An agglomeration multigrid method for unstructured grids. *Contemp. Math.*, 218:67–81, 1998.
- [5] L. P. Chew. Guaranteed-quality Delaunay meshing in 3D. In *Proc. 13th Symp. Comp. Geom.*, pages 391–393. ACM, 1997.
- [6] G. Constantinides and A. C. Payatakes. A Three Dimensional Network Model for Consolidated Porous Media. Basic Studies. *Chem. Eng. Comm.*, 81:55–81, 1980.
- [7] I. Fatt. The Network Model of Porous Media. *Trans. Am. Inst. Mem. Metall. Pet. Eng.*, 207:144–181, 1956.
- [8] D. Feuchter, I. Heppner, S. Sauter, and G. Wittum. Bridging the gap between geometric and algebraic multigrid methods (extended version). Technical report, Universität Zürich, 2002. Preprint no. 01-2002.

- [9] P. George. *Automatic Mesh Generation and Finite Element Computation*, volume IV, chapter Finite Element Methods (Part 2), pages 69–192. North-Holland, 1996. In: Handbook of Numerical Analysis, Eds.: P.G. Ciarlet and J.L. Lions.
- [10] L. Gibson and M. Ashby. *Cellular Solids, Structures and Properties*. Pergamon Press, Exeter, 1989.
- [11] M. L. Glasser and J. Boersma. Exact Values for the Cubic Lattice Green Functions. *J. Phys.*, 133:5017–5023, 2000.
- [12] M. Griebel and S. Knapek. A multigrid-homogenization method. In W. Hackbusch and G. Wittum, editors, *Modeling and Computation in Environmental Sciences*, pages 187–202, Braunschweig, 1997. Vieweg. Notes Numer. Fluid Mech. 59.
- [13] W. Hackbusch. A sparse matrix arithmetic based on \mathcal{H} -Matrices. Part I: Introduction to \mathcal{H} -Matrices. *Computing*, 62:89–108, 1999.
- [14] W. Hackbusch and B. Khoromskij. A sparse \mathcal{H} -Matrix Arithmetic. Part II: Applications to Multi-Dimensional Problems. *Computing*, 64(22):21–47, 2000.
- [15] W. Hackbusch, B. Khoromskij, and S. Sauter. On \mathcal{H}^2 -matrices. In H.-J. Bungartz, R. Hoppe, and C. Zenger, editors, *Lectures on Applied Mathematics*, pages 9–30, Heidelberg, 2000. Springer-Verlag.
- [16] W. Hackbusch and S. Sauter. Composite Finite Elements for Problems Containing Small Geometric Details. Part II: Implementation and Numerical Results. *Comput. Visual. Sci.*, 1(1):15–25, 1997.
- [17] J. C. Hansen, S. Chien, R. Skalog, and A. Hoger. A Classic Network Model Based on the Structure of the Red Blood Cell Membrane. *Biophys. J.*, 70:146–166, 1996.
- [18] G. S. Joyce. On the Simple Cubic Lattice Green Functions. *Proc. Roy. Soc., London Ser. A*, 445:463–477, 1994.
- [19] R. Kornhuber and H. Yserentant. Multilevel Methods for Elliptic Problems on Domains not Resolved by the Coarse Grid. *Contemporary Mathematics*, 180:49–60, 1994.
- [20] J. Mandel, M. Brezina, and P. Vaněk. Energy optimization of algebraic multigrid bases. *Computing*, 62:205–228, 1999.
- [21] P. G. Martinson. *Fast Multiscale Methods for Lattice Equations*. PhD thesis, University of Texas at Austin, 2002.
- [22] M. Ostoja-Starzewski. Lattice Models in Micromechanics. *App. Mech. Review*, 55(1):35–60, 2002.

- [23] M. Ostoja-Starzewski, P. Y. Shang, and K. Alzebdoh. Spring Network Models in Elasticity and Fractures of Composites and Polycrystals. *Comp. Math. Sci.*, 7:89–93, 1996.
- [24] G. I. Pshenichnov. *Theory of Lattice Plates and Shells*. World Scientific, Singapore, 1993.
- [25] J. Ruge and K. Stüben. Algebraic multigrid. In S. McCormick, editor, *Multigrid Methods*, pages 73–130, Pennsylvania, 1987. SIAM Philadelphia.
- [26] J. Shewchuk. Triangle:Engineering a 2D Quality Mesh Generator and Delaunay Triangulator. In *First Workshop on Appl. Geom.*, pages 124–133, Philadelphia, Pennsylvania, USA, 1996. Association for Computing Machinery.
- [27] J. Shewchuk. Tetrahedral Mesh Generation by Delaunay Refinement. In *Proc. Of the 14th Annual Symp. On Comp. Geom.*, pages 86–95, Minneapolis, USA, 1998. Association of Computing Machinery.
- [28] J. Xu. The auxiliary space method and optimal multigrid preconditioning techniques for unstructured grids. *Computing*, 56:215–235, 1996.